

Symmetry breaking and restoration using the equation-of-motion technique for nonequilibrium quantum impurity models

Tal J. Levy and Eran Rabani

School of Chemistry, The Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel

The description of the dynamics of correlated electrons in quantum impurity models is typically described within the nonequilibrium Green function formalism combined with a suitable approximation. One common approach is based on the equation-of-motion technique often used to describe different regimes of the dynamic response. Here, we show that this approach may violate certain symmetry relations that must be fulfilled by the definition of the Green functions. These broken symmetries can lead to unphysical behavior. To circumvent this pathological shortcoming of the equation-of-motion approach we provide a scheme to restore basic symmetry relations. Illustrations are given for the Anderson and double Anderson impurity models.

I. INTRODUCTION

Describing the transport of electrons through an interacting region is a challenging task and typically involves the calculation of the dynamics of correlated electrons driven away from equilibrium^{1–3}. In general, this many body out-of-equilibrium problem cannot be solved exactly but for a few simple cases^{4–7}. Excluding recent developments based on brute-force approaches such as time-dependent numerical renormalization-group techniques^{8–10}, iterative^{11–13} or stochastic^{14–18} diagrammatic techniques to real time path integral formulations, wave function based approaches¹⁹, or reduced dynamic approaches^{20,21}, all suitable to relatively simple model systems, most theoretical treatments of quantum transport rely on approximations of some sort. One well studied approach is based on the nonequilibrium Green function (NEGF) formalism otherwise known as the Keldysh NEGF or the Schwinger-Keldysh formalism^{22,23}, which is widely used to describe transport phenomena^{24–26}.

Based on the NEGF, an exact expression for the stationary current through an interacting system coupled to large non-interacting metallic leads in terms of the system's Green function can be derived²⁷:

$$I = \frac{ie}{2\pi\hbar} \int d\varepsilon (\text{Tr} \{ f_L(\varepsilon - \mu_L) \mathbf{\Gamma}_L(\varepsilon) \times (\mathbf{G}^r(\varepsilon) - \mathbf{G}^a(\varepsilon)) \} + \text{Tr} \{ \mathbf{\Gamma}_L \mathbf{G}^<(\varepsilon) \}), \quad (1)$$

or equivalently

$$I = \frac{e}{\hbar} \int d\varepsilon \text{Tr} \{ \mathbf{\Sigma}_L^<(\varepsilon) \mathbf{G}^>(\varepsilon) - \mathbf{\Sigma}_L^>(\varepsilon) \mathbf{G}^<(\varepsilon) \} \quad (2)$$

where \mathbf{G}^r (\mathbf{G}^a) is the retarded (advanced) Green function (GF) of the system, $\mathbf{G}^<$ ($\mathbf{G}^>$) is the lesser (greater) GF of the system, which will be defined later below. The lesser tunneling self-energy is given by $\mathbf{\Sigma}_{L0}^< = i f_L(\varepsilon - \mu_L) \mathbf{\Gamma}_L$, where $f_k(\varepsilon - \mu_k)$ is the Fermi-Dirac distribution and $\mathbf{\Gamma}_L$ is the matrix coupling the interacting system to the left reservoir with elements $(\mathbf{\Gamma}_L)_{mn} = 2\pi\rho_k(\varepsilon) t_{kn} t_{km}^*$ (t_{km} is the hopping matrix elements between the system and the left reservoir). The calculation of the system's GF required to obtain the current (or other observables) is

far from trivial, excluding simple noninteracting cases. Most applications are based on perturbative diagrammatic techniques to obtain \mathbf{G}^r , \mathbf{G}^a , $\mathbf{G}^<$ and $\mathbf{G}^>$ ²⁸. Alternatively, one can use the equation-of-motion (EOM) approach, which allows to deduce the system's GFs by deriving the corresponding equations of motion^{29–31}. In light of its simplicity, it has been used extensively to describe transport phenomena such as the Coulomb blockade³² and the Kondo effect^{30,33,34}, providing qualitative and in some cases quantitative results. When applied to interacting systems, the EOM for the GF gives rise to an infinite hierarchy of equations of higher-order GFs. A well-known approximation procedure is then to truncate this hierarchy, thus introducing a mean-field like description to some observables. These equations for the GFs then need to be solved self-consistently for the resulting closed set of equations. Although successful, the EOM technique has its drawbacks³⁵.

In this paper we show that while a closure can always be obtained, it is not clear a priori whether it fulfills symmetry relations that single particle GFs must obey. This failure can lead to solutions which are not physical, such as complex occupation of levels and even finite currents at zero bias. We also propose an approach to fix this deficiency by imposing a set of rules to reconstruct GFs that fulfill basic symmetry relations. Illustrations are given for the Anderson model³⁶ at the Kondo regime and for the double Anderson model³⁷. Our paper is organized as follows: in Sec. II we describe the EOM approach and the single site and double site Anderson models. In Sec. III we discuss symmetry relation for GFs and illustrate symmetry breaking for the aforementioned models with specific closures suitable to describe the Kondo effect. In Sec. IV we provide a recipe to restore the basic symmetry relations within the EOM approach and discuss implications for level occupancy and coherences, current, and sum rules for the Anderson model in the Kondo regime and the double Anderson model. Finally, in Sec. V we conclude.

II. EOM TECHNIQUE AND MODELS

A. Equations of motion

The EOM for the contour ordered GF³⁸ is obtained from the Heisenberg EOM for a Heisenberg operator $\frac{d}{dt}\hat{A}(t) = \frac{i}{\hbar} [\hat{H}(t), \hat{A}_H(t)] + \frac{\partial}{\partial t}\hat{A}_H(t)$, where in our case $\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$. Here \hat{H}_0 stands for the one body noninteracting part of $\hat{H}(t)$, $\hat{V}(t) = \hat{H}(t) - \hat{H}_0$, and $[\hat{A}, \hat{B}]$ is the commutator. Let us consider a generic example. We define the contour ordered GF

$$G(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) = -\frac{i}{\hbar} \langle T_C \hat{\Psi}_H(\mathbf{r}_2, t_2) \hat{\Psi}_H^\dagger(\mathbf{r}_1, t_1) \rangle, \quad (3)$$

where T_C is the contour time ordering operator and $\hat{\Psi}_H(\hat{\Psi}_H^\dagger)$ is the system's annihilation (creation) field operator in the Heisenberg picture (in what follows we omit the H index). The EOM³⁹ for $G(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1)$ can be written as (omitting the \mathbf{r} dependence for brevity)

$$\begin{aligned} G(t_2, t_1) &= g_2(t_2, t_1) \langle \{ \hat{\Psi}, \hat{\Psi}^\dagger \} \rangle \\ &\quad - \frac{i}{\hbar} \int_C dt g_2(t_2, t) \\ &\quad \times \langle T_C [\hat{\Psi}(t), \hat{V}(t)] \hat{\Psi}^\dagger(t_1) \rangle, \end{aligned} \quad (4)$$

where $(i\hbar \frac{\partial}{\partial t_2} - \varepsilon) g_2(t_2, t_1) = \delta(t_1 - t_2)$, $\{ \hat{A}, \hat{B} \}$ is the anti-commutator, and ε is defined from the equation, $\varepsilon \hat{\Psi}(t) = [\hat{\Psi}(t), \hat{H}_0]$. For example, if $\hat{H}_0 = \sum_n (\varepsilon_n - \mu) \hat{d}_n^\dagger \hat{d}_n$ and $\hat{\Psi} = \hat{d}_i$ then $\varepsilon = \varepsilon_i - \mu$. Following Langreth theorem⁴⁰, we can change the contour integration in equation (4) to integration along the real time axis. This yields (see Sec. III for the definitions of the different real-time GFs)

$$\begin{aligned} G^r(t_2, t_1) &= g_2^r(t_2, t_1) \langle \{ \hat{\Psi}, \hat{\Psi}^\dagger \} \rangle \\ &\quad + \int_{t_1}^{t_2} dt g_2^r(t_2, t) \mathbb{G}^r(t, t_1), \\ G^<(t_2, t_1) &= g_2^<(t_2, t_1) \langle \{ \hat{\Psi}, \hat{\Psi}^\dagger \} \rangle \\ &\quad + \int_{t_0}^{t_2} dt g_2^r(t_2, t) \mathbb{G}^<(t, t_1) \\ &\quad + \int_{t_0}^{t_1} dt g_2^<(t_2, t) \mathbb{G}^a(t, t_1), \end{aligned} \quad (5)$$

where $G^r(t_2, t_1)$ is the retarded GF usually used to calculate the response of the system at time t_2 to an earlier perturbation of the system at time t_1 . $G^<(t_2, t_1)$ is the lesser GF which plays the role of the single particle density matrix, and $\mathbb{G}(t_2, t_1) = -\frac{i}{\hbar} \langle T_C [\hat{\Psi}(t_2), \hat{V}(t_2)] \hat{\Psi}^\dagger(t_1) \rangle$ is a new GF generated by the EOM procedure. Depending on the Hamiltonian

it can be a single particle GF or a many particle GF and can involve lead operators as well as system operators. In steady state, the GFs depend only on the difference in time, $t = t_2 - t_1$, which is simpler to express in Fourier space

$$G^r(\omega) = g_2^r(\omega) \langle \{ \hat{\Psi}, \hat{\Psi}^\dagger \} \rangle + g_2^r(\omega) \mathbb{G}^r(\omega), \quad (6)$$

$$\begin{aligned} G^<(\omega) &= g_2^<(\omega) \langle \{ \hat{\Psi}, \hat{\Psi}^\dagger \} \rangle + g_2^r(\omega) \mathbb{G}^<(\omega) \\ &\quad + g_2^<(\omega) \mathbb{G}^a(\omega). \end{aligned} \quad (7)$$

To simplify the notation we denote the Fourier transform of $G(t_2 - t_1) = G(t)$ as $G(\omega)$, i.e., functions with an argument “ ω ” are Fourier transforms of their time-domain counterparts. At this stage one has to evaluate $\mathbb{G}(t_2, t_1)$ ($\mathbb{G}(t)$ in steady state). Except for very simple cases, where an exact closure can be obtained, writing the EOM for $\mathbb{G}(t_2, t_1)$ will produce new and/or “higher order” GFs that need to be evaluated. This leads (in principle) to an infinite set of equations. The idea of the EOM method is therefore, to truncate this hierarchy of equations making a mean-field like approximation for the “higher-order” GFs through lower order functions. This is the Achilles heel of this method as there is no systematic way to close the equations. Usually the approximations have physical meaning within the regime of the problem at hand^{33,41,42}. In what follows we demonstrate that different approximations can sometimes break symmetry relations that the GFs must fulfill. We will use two impurity models to demonstrate at what level of approximation the symmetry relations are violated and propose a scheme to restore symmetrization.

B. The impurity models

To illustrate the shortcomings of the EOM approach, we refer to the Anderson model^{33,36,43} and the double Anderson model³⁷ to represent two different degrees of complexity in correlated systems. As commonly used, we split the total Hamiltonian into three parts²⁸:

$$\hat{H} = \hat{H}_{sys} + \hat{H}_{bath} + \hat{H}_{int}, \quad (8)$$

where \hat{H}_{bath} describes the macroscopic leads (left and right contacts), \hat{H}_{sys} describes the system of interest (in our case the impurities), and \hat{H}_{int} is the interaction Hamiltonian between the system and the leads. The contacts (leads) are modeled as infinite non-interacting fermionic baths^{44–46} with a Hamiltonian in second quantization given by

$$\hat{H}_{bath} = \sum_{\sigma, k \in \{L, R\}} \epsilon_{k, \sigma} c_{k, \sigma}^\dagger c_{k, \sigma}, \quad (9)$$

where $\epsilon_{k, \sigma}$ is the energy of a free electron in the left (L) or right (R) lead, in momentum state k and spin σ . The operator $c_{k, \sigma}$ ($c_{k, \sigma}^\dagger$) is the annihilation (creation) operator

of such an electron. The form chosen for \hat{H}_{sys} depends on the system studied. For the Anderson impurity model³⁶

$$\hat{H}_{sys} = \sum_{\sigma \in \{\uparrow, \downarrow\}} \epsilon_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow}. \quad (10)$$

Here $n_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$ is the number operator of the spin σ electron with energy ϵ_{σ} and U is the repulsion energy between two electrons on the same site with opposite spins (intra-site repulsion). The second model we discuss is the double Anderson model³⁷

$$\begin{aligned} \hat{H}_{sys} = & \sum_{\sigma, m \in \{\alpha, \beta\}} \epsilon_{m\sigma} n_{m\sigma} + \sum_m U_m n_{m\uparrow} n_{m\downarrow} \\ & + \sum_{\sigma, \sigma'} V_{\alpha\beta}^{\sigma\sigma'} n_{\alpha\sigma} n_{\beta\sigma'} + \sum_{\sigma} [h_{\alpha\beta}^{\sigma} d_{\alpha}^{\dagger} d_{\beta} + h.c.], \end{aligned} \quad (11)$$

where the first two terms on the R.H.S are similar to the Anderson impurity model Hamiltonian (extended to 2 sites), $V_{\alpha\beta}^{\sigma\sigma'}$ is the repulsion energy between two electrons on different sites (inter-site repulsion), and $h_{\alpha\beta}^{\sigma}$ is the coupling strength for electron hopping between the two sites. The interaction between the system and the contacts is simply given by the tunneling Hamiltonian⁴⁷

$$\hat{H}_{int} = \sum_{m, \sigma, k \in \{L, R\}} t_{k, m}^{\sigma} c_{k, \sigma}^{\dagger} d_{m, \sigma} + h.c.. \quad (12)$$

The parameter $t_{k, m}^{\sigma}$ represents the coupling strength between the system and the leads, and the index m runs over the site index $\{\alpha, \beta\}$ in the double Anderson model.

III. SYMMETRY BREAKING IN IMPURITY MODELS

A. Definitions and symmetry relations

In the Keldysh formalism the two time NEGF is defined on a contour. In accordance with where on the contour the two times are placed one can define six real-time GFs⁴⁸; the time-ordered G^t , anti-time ordered $G^{\bar{t}}$, lesser $G^<$, greater $G^>$, retarded G^r , and advanced G^a :

$$\begin{aligned} G_{\alpha\beta}^t(t_2, t_1) &= -\frac{i}{\hbar} \theta(t_2 - t_1) \langle \hat{\Psi}_{\alpha}(t_2) \hat{\Psi}_{\beta}^{\dagger}(t_1) \rangle \\ &\quad + \frac{i}{\hbar} \theta(t_1 - t_2) \langle \hat{\Psi}_{\beta}^{\dagger}(t_1) \hat{\Psi}_{\alpha}(t_2) \rangle, \\ G_{\alpha\beta}^{\bar{t}}(t_2, t_1) &= -\frac{i}{\hbar} \theta(t_1 - t_2) \langle \hat{\Psi}_{\alpha}(t_2) \hat{\Psi}_{\beta}^{\dagger}(t_1) \rangle \\ &\quad + \frac{i}{\hbar} \theta(t_2 - t_1) \langle \hat{\Psi}_{\beta}^{\dagger}(t_1) \hat{\Psi}_{\alpha}(t_2) \rangle, \\ G_{\alpha\beta}^<(t_2, t_1) &= \frac{i}{\hbar} \langle \hat{\Psi}_{\beta}^{\dagger}(t_1) \hat{\Psi}_{\alpha}(t_2) \rangle, \\ G_{\alpha\beta}^>(t_2, t_1) &= -\frac{i}{\hbar} \langle \hat{\Psi}_{\alpha}(t_2) \hat{\Psi}_{\beta}^{\dagger}(t_1) \rangle, \\ G_{\alpha\beta}^r(t_2, t_1) &= -\frac{i}{\hbar} \theta(t_2 - t_1) \langle \{ \hat{\Psi}_{\alpha}(t_2), \hat{\Psi}_{\beta}^{\dagger}(t_1) \} \rangle, \\ G_{\alpha\beta}^a(t_2, t_1) &= \frac{i}{\hbar} \theta(t_1 - t_2) \langle \{ \hat{\Psi}_{\alpha}(t_2), \hat{\Psi}_{\beta}^{\dagger}(t_1) \} \rangle. \end{aligned} \quad (13)$$

The retarded GF can be used to calculate the response of the system at time t_2 to an earlier perturbation of the system at time t_1 and is proportional to the local density of states, while the lesser GF is also known as the particle propagator and plays the role of the single particle density matrix. From equation (1) it is obvious that in order to calculate the stationary current the retarded, advanced and lesser GFs are needed, thus, the current is expressed in terms of the local density of states and the occupation of the system. Using the given definitions it is clear that the following relations must hold:

$$\begin{aligned} G_{\alpha\beta}^r(t_2, t_1) &= (G_{\beta\alpha}^a(t_1, t_2))^*, \\ G_{\alpha\beta}^{<, >}(t_2, t_1) &= - (G_{\beta\alpha}^{<, >}(t_1, t_2))^*, \\ G_{\alpha\beta}^r(t_2, t_1) - G_{\alpha\beta}^a(t_2, t_1) &= G_{\alpha\beta}^>(t_2, t_1) - G_{\alpha\beta}^<(t_2, t_1). \end{aligned} \quad (14)$$

In steady state these relations can be rewritten in Fourier space as:

$$\begin{aligned} G_{\alpha\beta}^r(\omega) &= (G_{\beta\alpha}^a(\omega))^*, \\ G_{\alpha\beta}^{<, >}(\omega) &= - (G_{\beta\alpha}^{<, >}(\omega))^*, \\ G_{\alpha\beta}^r(\omega) - G_{\alpha\beta}^a(\omega) &= G_{\alpha\beta}^>(\omega) - G_{\alpha\beta}^<(\omega). \end{aligned} \quad (15)$$

In what follows we show that these relations do not hold when the GFs are obtained by the EOM technique with an arbitrary closure.

B. The Anderson model

Following the derivation in Refs. 28,33,47 we define the following contour ordered GF:

$$G_{\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C d_{\sigma}(t) d_{\sigma}^{\dagger}(t') \rangle, \quad (16)$$

$$G_2(t, t') = -\frac{i}{\hbar} \langle T_C n_{\bar{\sigma}}(t) d_{\sigma}(t) d_{\sigma}^{\dagger}(t') \rangle, \quad (17)$$

where $\bar{\sigma}$ is the opposite spin of σ . Various approximate decoupling procedures can be applied to the many particle GF⁴⁹. Here we follow the approximation scheme used in Refs. 28,33 where all electronic correlations containing at most one lead operator, are not decoupled and their EOM are calculated. Higher order GFs involving (opposite) spin correlations in the leads are set to zero, and the remaining higher order GFs involving lead and system degrees of freedom are decoupled such that $F_2(t, t') = -\frac{i}{\hbar} \langle T_C c_{kn\bar{\sigma}}^{\dagger}(t) d_{\sigma}(t) c_{qm\bar{\sigma}}(t) d_{\sigma}^{\dagger}(t') \rangle = -\delta_{kq} \delta_{mn} f_k(\epsilon_n - \mu_k) G_{\sigma\sigma}(t, t')$. The resulting EOMs (in Fourier space) are:

$$(\hbar\omega - \epsilon_{\sigma} - \Sigma_0(\omega)) G_{\sigma\sigma}(\omega) = 1 + U G_2(\omega), \quad (18)$$

$$\begin{aligned} G_2(\omega) &= (\hbar\omega - \epsilon_{\sigma} - U - \Sigma_0(\omega) - \Sigma_3(\omega))^{-1} \\ &\quad \times (\langle n_{\bar{\sigma}} \rangle - \Sigma_1(\omega) G_{\sigma\sigma}(\omega)), \end{aligned} \quad (19)$$

where $\langle n_{\bar{\sigma}} \rangle = -\frac{i\hbar}{2\pi} \int_{-\infty}^{\infty} G_{\bar{\sigma}\bar{\sigma}}^<(\omega) d\omega$, $\Sigma_0(\omega) = \sum_{i,k \in \{L,R\}} \frac{|t_{k\sigma}|^2}{\hbar\omega - \varepsilon_{k,i,\sigma}}$ is the exact self-energy for the non-interacting case, $\Sigma_1(\omega)$ and $\Sigma_3(\omega)$ are the self-energies due to the tunneling of the $\bar{\sigma}$ electron, and are given by

$$\Sigma_j(\omega) = \sum_{k \in \{L,R\}} A_k^{(j)} |t_{k\sigma}|^2 \times \left(\frac{1}{\hbar\omega + \varepsilon_{k,\bar{\sigma}} - \varepsilon_{\sigma} - \varepsilon_{\bar{\sigma}} - U} + \frac{1}{\hbar\omega - \varepsilon_{k,\bar{\sigma}} - \varepsilon_{\sigma} + \varepsilon_{\bar{\sigma}}} \right), \quad j = 1, 3 \quad (20)$$

with $A_k^{(1)} = f_k(\varepsilon_{k,\sigma} - \mu_k)$, $A_k^{(3)} = 1$, and $f_k(\varepsilon_{k,\sigma} - \mu_k)$ is the Fermi Dirac distribution. To show that these set of equations break the symmetry relation $G_{\sigma\sigma}^<(\omega) = -(G_{\sigma\sigma}^<(\omega))^*$ we define

$$\Sigma_4(\omega) = \Sigma_0(\omega) + \Sigma_3(\omega), \quad (21)$$

$$g(\omega) = \frac{1}{\hbar\omega - \varepsilon_{\sigma} - \Sigma_0(\omega)}, \quad (22)$$

$$g_2(\omega) = \frac{1}{\hbar\omega - \varepsilon_{\sigma} - U - \Sigma_4(\omega)}. \quad (23)$$

With these definitions equations (18) and (19) can be rewritten (omitting (ω) for brevity) as:

$$G_{\sigma\sigma} = g + gUG_2, \quad (24)$$

$$G_2 = g_2 \langle n_{\bar{\sigma}} \rangle - g_2 \Sigma_1 G_{\sigma\sigma}. \quad (25)$$

Substituting equation (25) in equation (24) and applying the Langreth rules we find that the lesser GF is given by

$$\begin{aligned} G_{\sigma\sigma}^< &= g^< + g^r U P^r g_2^< \langle n_{\bar{\sigma}} \rangle + g^< U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle - \Sigma_1^a g^a) \\ &- g^r U P^r g_2^r (\Sigma_1^r g^< + \Sigma_1^< g^a) - g^r U P^r g_2^< \Sigma_1^a g^a \\ &- g^r U P^r g_2^r \Sigma_1^r g^< U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle + \Sigma_1^a g^a) \\ &- g^r U P^r g_2^r \Sigma_1^< g^a U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle + \Sigma_1^a g^a) \\ &- g^r U P^r g_2^< \Sigma_1^a g^a U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle + \Sigma_1^a g^a), \end{aligned} \quad (26)$$

where $P^{r,a} = \frac{1}{1 + g_2^{r,a} \Sigma_1^{r,a} g^{r,a} U}$, $g^< = g^r \Sigma_0^< g^a$, and $g_2^< = g_2^r \Sigma_4^< g_2^a$. Applying the principle of reductio ad absurdum we assume $G_{\sigma\sigma}^<$ is imaginary. Since it must hold for any real value of $\langle n_{\bar{\sigma}} \rangle$ between 0 and 1, we argue that the term

$$\begin{aligned} A_1 &= g^r U P^r g_2^< \langle n_{\bar{\sigma}} \rangle + g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle \\ &- g^r U P^r g_2^r \Sigma_1^r g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle \\ &- g^r U P^r g_2^r \Sigma_1^< g^a U P^a g_2^a \langle n_{\bar{\sigma}} \rangle \\ &- g^r U P^r g_2^< \Sigma_1^a g^a U P^a g_2^a \langle n_{\bar{\sigma}} \rangle, \end{aligned} \quad (27)$$

must be imaginary. Moreover, Since A_1 must be imaginary for any value of U the term

$$A_2 = g^r U P^r g_2^< \langle n_{\bar{\sigma}} \rangle + g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle, \quad (28)$$

should be imaginary as well. Using the fact that U and $\langle n_{\bar{\sigma}} \rangle$ are real quantities and by definition $g_2^<$ and $g^<$ are imaginary, for A_2 to be imaginary the following must hold:

$$\text{Im}(g^r P^r) g_2^< = -\text{Im}(P^a g_2^a) g^<, \quad (29)$$

or in other words, we demand that $\Re(A_2) = 0$. One can then show (see online supporting material for more information) that, in fact, the equality in equation (29) does not hold, namely, $G_{\sigma\sigma}^<(\omega)$ is not an imaginary function and the relation $G_{\sigma\sigma}^<(\omega) = -(G_{\sigma\sigma}^<(\omega))^*$ is not satisfied. In turn, this implies that $\langle n_{\sigma} \rangle$ (the occupation number) is a complex number, which of course is not physical. Following the same derivation one can show that $G_{\sigma\sigma}^>(\omega)$ is not an imaginary function either. All the other relations given in equation (15) are fulfilled.

If one is only interested in the Coulomb blockade regime, it is not necessary to go to the level of approximation presented here (which is essential to obtain the Kondo effect). For the Coulomb blockade regime one can turn to the approximation presented in Refs. 32, where on top of the approximations described above we also neglect the simultaneous hopping of electron pairs to and from the system. This approximation does not violate the symmetry relations of the single particle GF (see online supporting information for further discussion), but as pointed above, it does not reproduce the Kondo peaks at low temperatures.

C. The double Anderson model

For the double Anderson model we follow the derivation given in Ref. 50, and define the following contour ordered GF

$$G_{\alpha\beta}^{\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C d_{\alpha\sigma}(t) d_{\beta\sigma}^\dagger(t') \rangle, \quad (30)$$

$$\mathbb{G}_{\alpha\beta\gamma}^{\tau\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C n_{\alpha\tau}(t) d_{\beta\sigma}(t) d_{\gamma\sigma}^\dagger(t') \rangle, \quad (31)$$

where $\tau = \sigma, \bar{\sigma}$. The approximations used in Ref. 50 are: (a) neglect the simultaneous hopping of electron pairs to and from the system, (b) assume that $F_2(t, t') = -\frac{i}{\hbar} \langle T_C c_{k\sigma}(t) n(t) d_{\beta\sigma}^\dagger(t') \rangle \approx -\frac{i}{\hbar} \sum_{\gamma=\alpha,\beta} t_{k,\gamma}^\sigma \int dt_1 g_k(t, t_1) \langle T_C d_{\gamma\sigma}(t_1) n(t_1) d_{\beta\sigma}^\dagger(t') \rangle$ where $n(t)$ is the number operator of one of the electrons of the system, and $(i\hbar \frac{\partial}{\partial t} - \varepsilon_{k\sigma}) g_k(t, t_1) = \delta(t - t_1)$, and (c) higher order GFs of the form $-\frac{i}{\hbar} \langle T_C [n_{\gamma,\sigma}(t) n_{\delta,\tau}(t) d_{\alpha,\sigma}(t) d_{\beta,\sigma}^\dagger(0)] \rangle$ are decoupled to $-\frac{i}{\hbar} \langle n_{\gamma,\sigma}(t) \rangle \langle T_C n_{\delta,\tau}(t) d_{\alpha,\sigma}(t) d_{\beta,\sigma}^\dagger(0) \rangle - \frac{i}{\hbar} \langle n_{\delta,\sigma}(t) \rangle \langle T_C n_{\gamma,\sigma}(t) d_{\alpha,\sigma}(t) d_{\beta,\sigma}^\dagger(0) \rangle$. These approxi-

mations lead to the following results

$$\begin{aligned}
G_{\alpha\beta}^{\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha,\sigma} - \Sigma_0(\omega))^{-1} \times (\delta_{\alpha\beta}^{\sigma\sigma} \\
&+ h_{\alpha\beta}^{\sigma} G_{\beta\beta}^{\sigma\sigma}(\omega) + U_{\alpha} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) \\
&+ V_{\alpha\beta}^{\sigma\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\alpha\beta}^{\sigma\sigma} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega)),
\end{aligned} \tag{32}$$

$$\begin{aligned}
\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha\sigma} - U_{\alpha} - V_{\alpha\beta}^{\sigma\sigma} \langle n_{\beta\sigma} \rangle - V_{\alpha\beta}^{\sigma\bar{\sigma}} \langle n_{\beta\bar{\sigma}} \rangle - \Sigma_0(\omega))^{-1} \\
&\times [h_{\alpha\beta}^{\sigma} \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\alpha\bar{\sigma}} \rangle (V_{\alpha\beta}^{\sigma\sigma} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega) + V_{\alpha\beta}^{\sigma\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \\
\mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\beta\sigma} - U_{\beta} \langle n_{\beta\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\sigma} \langle n_{\alpha\sigma} \rangle - V_{\beta\alpha}^{\sigma\bar{\sigma}} - \Sigma_0(\omega))^{-1} \\
&\times [\langle n_{\alpha\bar{\sigma}} \rangle + h_{\beta\alpha}^{\sigma} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\alpha\bar{\sigma}} \rangle (U_{\beta} \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\beta\alpha}^{\sigma\sigma} \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega))], \\
\mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\beta\sigma} - U_{\beta} \langle n_{\beta\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\bar{\sigma}} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\sigma} - \Sigma_0(\omega))^{-1} \\
&\times [\langle n_{\alpha\sigma} \rangle + h_{\beta\alpha}^{\sigma} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega) + \langle n_{\alpha\sigma} \rangle (U_{\beta} \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\beta\alpha}^{\sigma\bar{\sigma}} \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \\
\mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha\sigma} - U_{\alpha} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\alpha\beta}^{\sigma\sigma} \langle n_{\beta\sigma} \rangle - V_{\alpha\beta}^{\sigma\bar{\sigma}} - \Sigma_0(\omega))^{-1} \\
&\times [h_{\alpha\beta}^{\sigma} \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\beta\bar{\sigma}} \rangle (U_{\alpha} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\alpha\beta}^{\sigma,\sigma} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega))], \\
\mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha\sigma} - U_{\alpha} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\alpha\beta}^{\sigma\bar{\sigma}} \langle n_{\beta\bar{\sigma}} \rangle - V_{\alpha\beta}^{\sigma\sigma} - \Sigma_0(\omega))^{-1} \\
&\times [-\langle d_{\beta\sigma}^{\dagger} d_{\alpha,\sigma} \rangle + h_{\alpha\beta}^{\sigma} \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega) + \langle n_{\beta,\sigma} \rangle (U_{\alpha} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\alpha,\beta}^{\sigma,\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \\
\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\beta\sigma} - U_{\beta} - V_{\beta\alpha}^{\sigma\bar{\sigma}} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\sigma} \langle n_{\alpha\sigma} \rangle - \Sigma_0(\omega))^{-1} \\
&\times [\langle n_{\beta\bar{\sigma}} \rangle + h_{\beta\alpha}^{\sigma} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\beta\bar{\sigma}} \rangle (V_{\beta\alpha}^{\sigma,\sigma} \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega) + V_{\beta\alpha}^{\sigma,\bar{\sigma}} \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega))],
\end{aligned} \tag{33}$$

We now show that given this set of equations, the symmetry relation $(G_{\alpha\beta}^{\sigma\sigma}(\omega))^r = ((G_{\beta\alpha}^{\sigma\sigma}(\omega))^a)^*$ is not satisfied. By applying the Langreth rules we can find the retarded and advanced projections of the single particle GF (equation (32)). For simplicity we derived them for the case where $V_{ij}^{\sigma\tau} = 0$. Define

$$(g_i)^{r,a} = \frac{1}{\hbar\omega - \varepsilon_{i,\sigma} - \Sigma_0^{r,a}}, \tag{34}$$

$$(g_{ii}^{\bar{\sigma}\sigma})^{r,a} = \frac{1}{\hbar\omega - \varepsilon_{i,\sigma} - U_i - \Sigma_0^{r,a}}, \tag{35}$$

$$(g_{ij}^{\bar{\sigma}\sigma})^{r,a} = \frac{1}{\hbar\omega - \varepsilon_{j,\sigma} - U_j \langle n_{j,\bar{\sigma}} \rangle - \Sigma_0^{r,a}}. \tag{36}$$

Given these definitions, the retarded and advanced GFs are given by:

$$\begin{aligned}
(G_{\alpha\beta}^{\sigma\sigma})^r &= (I - (g_{\alpha})^r h_{\alpha\beta}^{\sigma} (g_{\beta})^r h_{\beta,\alpha}^{\sigma})^{-1} \\
&\times ((g_{\alpha})^r h_{\alpha\beta}^{\sigma} (g_{\beta})^r + (g_{\alpha})^r h_{\alpha\beta}^{\sigma} (g_{\beta})^r U_{\beta} (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r + (g_{\alpha})^r U_{\alpha} (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r),
\end{aligned} \tag{37}$$

$$\begin{aligned}
(\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r &= (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha\bar{\sigma}} \rangle U_{\beta} \\
&\times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma})^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_{\alpha})^{-1} \\
&\times ((g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha\bar{\sigma}} \rangle + (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha\bar{\sigma}} \rangle U_{\beta} \\
&\times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma})^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle),
\end{aligned} \tag{38}$$

$$\begin{aligned}
(\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r &= (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_{\alpha} \\
&\times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma})^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha\bar{\sigma}} \rangle U_{\beta})^{-1} \\
&\times ((g_{\beta\beta}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle + (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_{\alpha} \\
&\times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^{\sigma})^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha\bar{\sigma}} \rangle),
\end{aligned} \tag{39}$$

$$\begin{aligned}
(G_{\beta\alpha}^{\sigma\sigma})^a &= (I - (g_{\beta})^a h_{\beta\alpha}^{\sigma} (g_{\alpha})^a h_{\alpha\beta}^{\sigma})^{-1} \\
&\times ((g_{\beta})^a h_{\beta\alpha}^{\sigma} (g_{\alpha})^a + (g_{\beta})^a h_{\beta\alpha}^{\sigma} (g_{\alpha})^a U_{\alpha} (\mathbb{G}_{\alpha\alpha\alpha}^{\bar{\sigma}\sigma\sigma})^a + (g_{\beta})^a U_{\beta} (\mathbb{G}_{\beta\beta\alpha}^{\bar{\sigma}\sigma\sigma})^a),
\end{aligned} \tag{40}$$

$$\begin{aligned}
(\mathbb{G}_{\beta\beta\alpha}^{\bar{\sigma}\sigma\sigma})^a &= (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta\bar{\sigma}} \rangle U_{\alpha} \\
&\times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma})^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle U_{\beta})^{-1} \\
&\times ((g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta\bar{\sigma}} \rangle + (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta\bar{\sigma}} \rangle U_{\alpha} \\
&\times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma})^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle),
\end{aligned} \tag{41}$$

$$\begin{aligned}
(\mathbb{G}_{\alpha\alpha\alpha}^{\bar{\sigma}\sigma\sigma})^a &= (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle U_{\beta} \\
&\times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma})^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta\bar{\sigma}} \rangle U_{\alpha})^{-1} \\
&\times ((g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle + (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma} (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle U_{\beta} \\
&\times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^{\sigma})^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^{\sigma} (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta\bar{\sigma}} \rangle).
\end{aligned} \tag{42}$$

Substituting the equations for $(\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega))^r$, $(\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega))^r$, $(\mathbb{G}_{\beta\beta\alpha}^{\bar{\sigma}\sigma\sigma}(\omega))^a$ and $(\mathbb{G}_{\alpha\alpha\alpha}^{\bar{\sigma}\sigma\sigma}(\omega))^a$ into equations (37) and (40), respectively, and comparing the resulting expressions we find that $(G_{\alpha\beta}^{\sigma\sigma}(\omega))^r \neq ((G_{\beta\alpha}^{\sigma\sigma}(\omega))^a)^*$ (see online supporting material for more details). Moreover, we find that none of the symmetry relations in equation (15) hold. In the following section we propose a symmetrization scheme that restores all the symmetries of the single particle GF.

IV. SYMMETRY RESTORATION

A. Guidelines to restore symmetry

The customary route to calculate the NEGF is as follows: (a) calculate the retarded GF and use it to obtain the advanced GF (by demanding $G_{\alpha\beta}^a(\omega) = (G_{\beta\alpha}^r(\omega))^*$). (b) Calculate the lesser/greater GF and symmetrize the lesser/greater to fulfill the quantum Onsager relations⁵¹, hence obeying $G_{\alpha\beta}^{<,>}(\omega) = - (G_{\beta\alpha}^{<,>}(\omega))^*$. In most applications of NEGF the advanced GF is not directly calculated and thus, the symmetry breakage does not always stand out. In fact, this common procedure restores the relation between the advanced and retarded GF and between the lesser/greater and their complex conjugate, but does not necessarily restore the relation $G_{\alpha\beta}^r(\omega) - G_{\alpha\beta}^a(\omega) = G_{\alpha\beta}^>(\omega) - G_{\alpha\beta}^<(\omega)$.

It can be shown that violation of the latter leads to violation of the fluctuation dissipation relation, $\mathbf{G}^< = -f_{eq}(\varepsilon - \mu_{eq})(\mathbf{G}^r - \mathbf{G}^a)$, at equilibrium. This oversimplified procedure can result in different values for the currents depending on how it is calculated, cf. equation (1) or equation (2). It may also lead to finite currents at zero-bias voltage (see Sec. IV C for more), which is physically incorrect.

In order to restore the symmetry relations that are imposed by the definitions of the GF (cf. equation 15), we suggest the following procedure:

1. Calculate the retarded/advanced GFs matrices ($\mathbf{G}^r/\mathbf{G}^a$) separately and use them to define “new” retarded/advanced GFs matrices $\tilde{\mathbf{G}}^r = \frac{1}{2}(\mathbf{G}^r + (\mathbf{G}^a)^\dagger)$ and $\tilde{\mathbf{G}}^a = \frac{1}{2}(\mathbf{G}^a + (\mathbf{G}^r)^\dagger) = (\tilde{\mathbf{G}}^r)^\dagger$.
2. Use the “new” retarded/advanced GFs matrices ($\tilde{\mathbf{G}}^r/\tilde{\mathbf{G}}^a$) to calculate the lesser/greater GFs matrices ($\mathbf{G}^</\mathbf{G}^>$). Again, use them to define “new” lesser/greater GFs matrices $\tilde{\mathbf{G}}^{<,>} = \frac{1}{2}(\mathbf{G}^{<,>} - (\mathbf{G}^{<,>})^\dagger)$.
3. Calculate the two anti-Hermitian matrices $\mathbf{A} = \tilde{\mathbf{G}}^> - \tilde{\mathbf{G}}^<$ and $\mathbf{B} = \tilde{\mathbf{G}}^r - \tilde{\mathbf{G}}^a$. Define the difference anti-Hermitian matrix $\mathbf{C} = \mathbf{A} - \mathbf{B}$, and redefine the retarded and advanced GFs $\tilde{\mathbf{G}}^r = \tilde{\mathbf{G}}^r + \frac{\mathbf{C}}{2}$, and $\tilde{\mathbf{G}}^a = \tilde{\mathbf{G}}^a - \frac{\mathbf{C}}{2}$.

The resulting GFs ($\tilde{\mathbf{G}}^r$, $\tilde{\mathbf{G}}^a$, $\tilde{\mathbf{G}}^<$ and $\tilde{\mathbf{G}}^>$) obey all symmetry relations of equation (15) by construction. Note that if the original GFs obeyed the symmetry relations to begin with, our symmetrization procedure will not alter them in any way.

We now turn to perform detailed calculations for both the Anderson and double Anderson models. For the Anderson model, we use the closure described in Sec. III B while for the double Anderson model we use the closure described in Sec. III C. The resulting EOMs were solved self-consistently in Fourier space with a frequency discretization of $N_\omega = 2^{14} - 2^{16}$ depending on the model parameters. Typically, < 15 self-consistent iterations were needed to converge the results. Convergence was declared when the population values at subsequent iteration steps did not change within a predefined tolerance value chosen as 10^{-6} . For each set of calculations we have applied the above symmetrization scheme and compared the results to those obtained without restoring symmetry, as detailed for each model.

B. Anderson impurity model

First, we address the effects of symmetry breakage in the Anderson model. The closure used is sufficient to describe the appearance of the Kondo resonances at low

temperatures, as seen in the upper panel of figure 1, where we plot the density of states as a function of energy for several temperatures, all calculated with symmetry restoration. The development of Kondo peaks in the density of states as the temperature decreases is clearly evident, signifying a regime of strong correlations which is qualitatively captured by the simple EOM approach when symmetry is restored.

In the lower panel of figure 1 we show one of the main flaws of the EOM approach for the Anderson impurity model, where we plot the value of $\langle n_\uparrow \rangle$ as a function of the source drain bias voltage with and without symmetry restoration. The most notable effect is the appearance of an imaginary portion to $\langle n_\uparrow \rangle$ as the source drain bias voltage is increased. To obtain the results, without symmetry restoration, only the real part of $\langle n_\sigma \rangle$ was used to converge the self-consistent equations for the GFs. By applying the symmetrization scheme proposed in Sec. IV A to the lesser GF calculated in Sec. III B, we restore the relation $G_{\alpha\beta}^{<,>}(\omega) = -\left(G_{\beta\alpha}^{<,>}(\omega)\right)^*$. This is sufficient to obtain a real value for $\langle n_\uparrow \rangle$, as clearly shown in the lower panel of figure 1. All other symmetry relation are not violated here and thus, our symmetrization procedure does not affect them at all. Interestingly, taking only the real part of $\langle n_\sigma \rangle$ provides identical results when compared to the results obtained after the full symmetrization procedure. However, this is only true for the simple case of the single site impurity model and does not hold for more complex systems.

C. The double Anderson model

We now turn to discuss the impact of symmetry breaking for the double Anderson model. This system is more involved compared to the single site Anderson model and thus, the level of closure used is somewhat simpler, as explained in Sec. III C. While for the case of a single site Anderson model only the relation $G_{\alpha\beta}^{<,>}(\omega) = -\left(G_{\beta\alpha}^{<,>}(\omega)\right)^*$ breaks down, in the double Anderson model we find that all 3 symmetries described by equation 15 are violated. This can be traced to the more complex form of the Hamiltonian for the double Anderson model, where each site is only coupled to one of the leads and transport is enabled by the direct hopping term between the two sites.

Similar to the case of the Anderson model, as a result of symmetry breaking the occupation of the levels $\langle n_{\alpha\sigma} \rangle$ is a complex number. In addition, the coherences, $\rho_{\alpha\beta}^{\sigma\sigma} = -\frac{i\hbar}{2\pi} \int_{-\infty}^{\infty} \left(G_{\alpha\beta}^{\sigma\sigma}(\omega)\right)^< d\omega$, should also fulfill certain symmetry relations, such as $\rho_{\alpha\beta}^{\sigma\sigma} = \left(\rho_{\beta\alpha}^{\sigma\sigma}\right)^*$. In figure 2 we plot the real and imaginary parts of $\rho_{\alpha\beta}^{\sigma\sigma}$ and $\rho_{\beta\alpha}^{\sigma\sigma}$ for the case where the symmetry procedure has been applied (left panels) and for the bare case (right panels). The upper panels show the imaginary part of $\rho_{\alpha\beta}^{\sigma\sigma}$

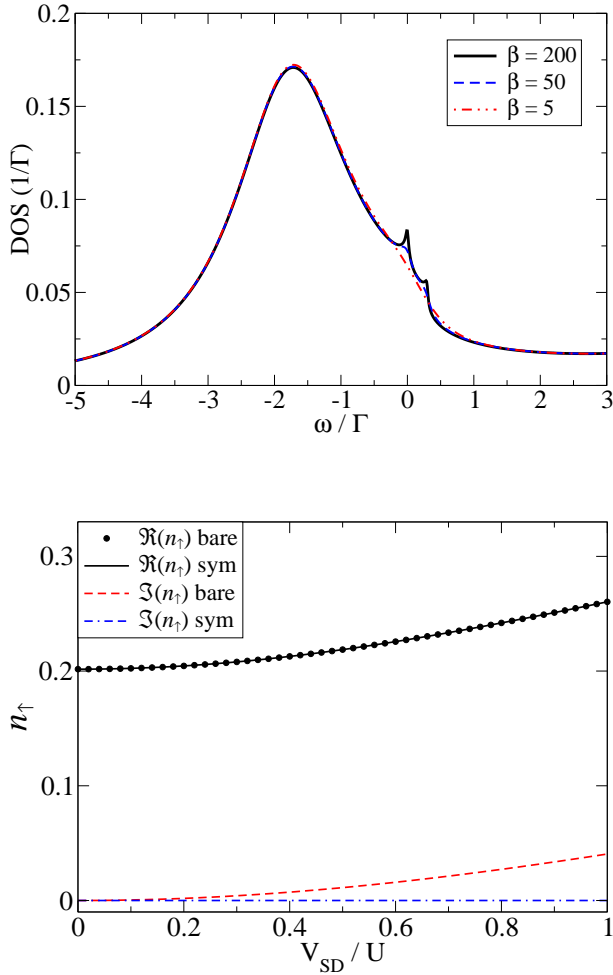


Figure 1: Upper panel: Density of states in the Kondo regime for nonequilibrium situation of the spin up electron after symmetrization for different temperatures. Parameters used are similar to those used in Refs. 34,52 (in units of $\Gamma = \Gamma_L + \Gamma_R$): $\mu_L = 3/10$, $\mu_R = 0$, $\varepsilon_{\downarrow,\uparrow} = -2$, and $U = 10$. The bands are modeled as a Lorentzian with a half bandwidth 100. Lower panel: Occupation of the spin up electron before (“bare”) and after (“sym”) symmetrization. As can be clearly seen the real part of the observable $\langle n_\uparrow \rangle$ is not affected by the symmetrization, and only the non physical imaginary part disappears. Parameters used (in units of U): $\Gamma_{L,\uparrow} = \Gamma_{R,\uparrow} = 0.3$, $\Gamma_{L,\downarrow} = \Gamma_{R,\downarrow} = 0.05$, $\varepsilon_\uparrow = 0.2$, $\varepsilon_\downarrow = -0.2$, $\beta = 4$ and $U = 1$.

and $\rho_{\beta\alpha}^{\sigma\sigma}$, which should show a mirror reflection about the zero axis (shown as thin solid line). This is, indeed, the case when symmetry is restored, however, it is destroyed when symmetry breaks down, in particular as the source drain bias increases. A more dramatic effect is shown for the real part of $\rho_{\alpha\beta}^{\sigma\sigma}$ and $\rho_{\beta\alpha}^{\sigma\sigma}$ (lower panels). The two curves representing $\Re(\rho_{\alpha\beta}^{\sigma\sigma})$ and $\Re(\rho_{\beta\alpha}^{\sigma\sigma})$ should be identical (left panel when symmetry is restored) but are quite distinct when symmetry is not obeyed (right panel).

In figure 3 we plot the current as a function of the source drain bias voltage for the double Anderson model. The current can be obtained from equation (1) (dashed

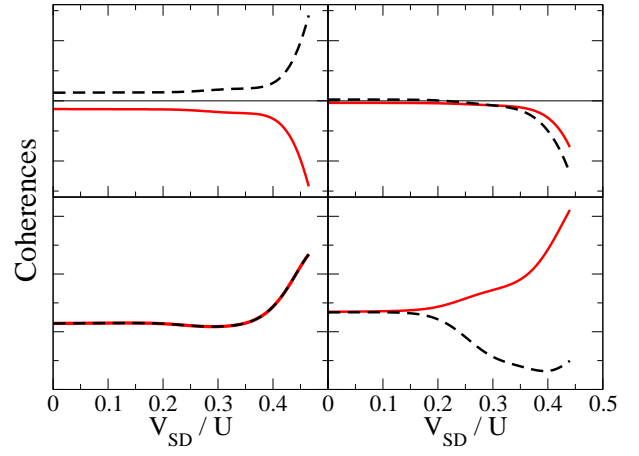


Figure 2: The imaginary (upper panels) and real (lower panels) parts of $\rho_{\alpha\beta}^{\sigma\sigma} = \langle d_{\beta\sigma}^\dagger d_{\alpha\sigma} \rangle$ (dashed line) and $\rho_{\beta\alpha}^{\sigma\sigma} = \langle d_{\alpha\sigma}^\dagger d_{\beta\sigma} \rangle$ (solid line) calculated before (right panels) and after (left panels) symmetry was restored. The solid thin line in the upper panels marks the zero axis. As expected, after symmetry restoration (left panels), $\Im(\rho_{\alpha\beta}^{\sigma\sigma}) = -\Im(\rho_{\beta\alpha}^{\sigma\sigma})$ and $\Re(\rho_{\alpha\beta}^{\sigma\sigma}) = \Re(\rho_{\beta\alpha}^{\sigma\sigma})$, while before symmetry restoration (right panels) these equalities are violated. Parameters used for the simulations in units of $U = U_\alpha = U_\beta$ are: $\Gamma_{\alpha\uparrow}^L = \Gamma_{\alpha\downarrow}^L = \Gamma_{\beta\uparrow}^R = \Gamma_{\beta\downarrow}^R = 0.0025$, $\Gamma_{\alpha\uparrow}^R = \Gamma_{\alpha\downarrow}^R = \Gamma_{\beta\uparrow}^L = \Gamma_{\beta\downarrow}^L = 0$, $h_{\alpha\beta}^\sigma = h_{\alpha\beta}^{\bar{\sigma}} = 0.25$, $V_{\alpha\beta}^{\sigma\tau} = 0.1$, $\varepsilon_{\alpha\uparrow} = \varepsilon_{\alpha\downarrow} = 0.1$, $\varepsilon_{\beta\uparrow} = \varepsilon_{\beta\downarrow} = -0.175$ and $\beta = 80$.

line) or from equation (2) (dotted curve). In the limit of infinite hierarchy in the EOM approach the two formulas should coincide. However, when approximations are introduced or when the hierarchy is truncated, the calculation of the current based on the two different formulas will coincide only if the symmetry relation $(G_{\alpha\beta}^{\sigma\tau}(\omega))^r - (G_{\alpha\beta}^{\sigma\tau}(\omega))^a = (G_{\alpha\beta}^{\sigma\tau}(\omega))^> - (G_{\alpha\beta}^{\sigma\tau}(\omega))^<$ is preserved. Indeed, in the case of a single site Anderson model, even if symmetry is not restored, this relation holds and the two calculations yield identical values for the current. However, in the present case, all 3 symmetry relations are broken and thus, equations (1) and (2) give different results for the current, as clearly evident in figure 3. More significantly is the fact that equation (1) produces a finite value for the current even when the bias is zero, indicating the break down of the fluctuation dissipation relation. When symmetry is restored (solid curve) the two calculations are identical, as they should be, and the violation of the fluctuation dissipation relation is also resolved.

The symmetrization scheme proposed here is not a “magic cure” and, in fact, does not resolve all issues of matter. It is well known that the lesser and greater GFs should obey a simple sum rule where the integral over the difference of their diagonal elements should always sum to 1:

$$S_{\alpha\sigma} = \frac{-i\hbar}{2\pi} \int d\varepsilon ((G_{\alpha\alpha}^{\sigma\sigma}(\varepsilon))^< - (G_{\alpha\alpha}^{\sigma\sigma}(\varepsilon))^>) = 1. \quad (43)$$

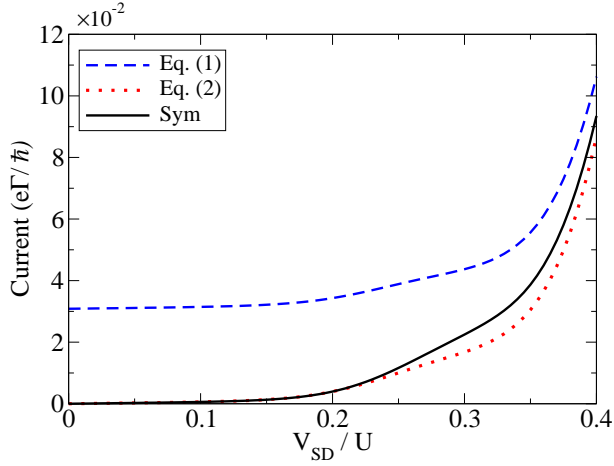


Figure 3: I-V curves calculated using equations (1) and (2) before (dashed and dotted lines) and after (solid line) applying the symmetry procedure suggested in Sec. IV A. As can be clearly seen, before symmetrization, calculating the current via the two different but equivalent formulas provide different results, one of which is not physical (dashed line) as the current is finite for $V_{SD} = 0$. The latter result suggests that the “unsymmetrized” GFs obtained through the EOM disobey the fluctuation dissipation relation. Parameters used for the simulations in units of $U = U_\alpha = U_\beta$ are: $\Gamma_{\alpha\uparrow}^L = \Gamma_{\alpha\downarrow}^L = \Gamma_{\beta\uparrow}^R = \Gamma_{\beta\downarrow}^R = 0.0025$, $\Gamma_{\alpha\uparrow}^R = \Gamma_{\alpha\downarrow}^R = \Gamma_{\beta\uparrow}^L = \Gamma_{\beta\downarrow}^L = 0$, $h_{\alpha\beta}^\sigma = h_{\alpha\beta}^{\bar{\sigma}} = 0.25$, $V_{\alpha\beta}^{\sigma\tau} = 0.1$, $\varepsilon_{\alpha\uparrow} = \varepsilon_{\alpha\downarrow} = 0.1$, $\varepsilon_{\beta\uparrow} = \varepsilon_{\beta\downarrow} = -0.175$ and $\beta = 80$.

In figure 4 we plot the sum rule as given by equation (43) for the double Anderson model where symmetry has been restored. A similar plot for the single site Anderson model yields a value of 1 regardless of whether symmetry has been restored or not within the closure discussed above. However, in the case of the more evolved double Anderson model, even when symmetry is restored and the GFs obey all 3 relations described in equation (15), the sum rule is violated. Nonetheless, the sum $\sum_{\alpha\sigma} S_{\alpha\sigma} = N_e$, where N_e is the total number of electrons in the system at maximal occupancy, is indeed preserved when symmetrization is restored.

V. SUMMARY

In this paper we have addressed the problem of symmetry breaking and restoring in the EOM approach to NEGF formalism. This formalism is based on deriving a hierarchy of equations of motion for the system’s Green functions and truncating this hierarchy at a desired (or tractable) order. Despite the uncontrolled approximation introduced by an arbitrary truncation, the closed set of equations is often used to describe the complex dynamics of correlated systems, including the Coulomb blockade and Kondo effect.

One shortcoming of the EOM approach, which has

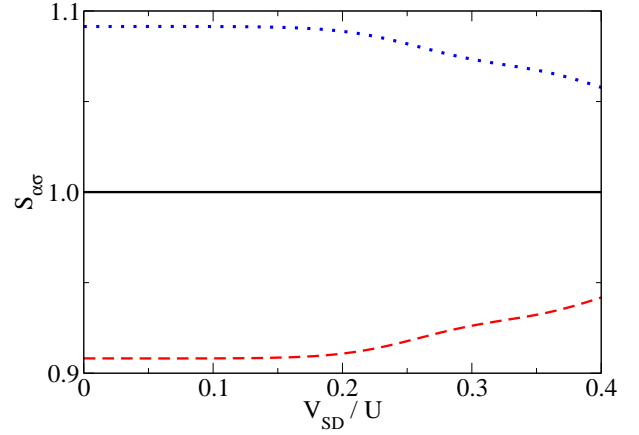


Figure 4: $S_{\alpha\sigma}$ (dashed line) and $S_{\beta\sigma}$ (dotted line) calculated from the “symmetrized” lesser and greater GFs as a function of the source drain bias voltage. The exact result should have been 1 (as marked by the solid line). Parameters used for the simulations in units of $U = U_\alpha = U_\beta$ are: $\Gamma_{\alpha\uparrow}^L = \Gamma_{\alpha\downarrow}^L = \Gamma_{\beta\uparrow}^R = \Gamma_{\beta\downarrow}^R = 0.0025$, $\Gamma_{\alpha\uparrow}^R = \Gamma_{\alpha\downarrow}^R = \Gamma_{\beta\uparrow}^L = \Gamma_{\beta\downarrow}^L = 0$, $h_{\alpha\beta}^\sigma = h_{\alpha\beta}^{\bar{\sigma}} = 0.25$, $V_{\alpha\beta}^{\sigma\tau} = 0.1$, $\varepsilon_{\alpha\uparrow} = \varepsilon_{\alpha\downarrow} = 0.1$, $\varepsilon_{\beta\uparrow} = \varepsilon_{\beta\downarrow} = -0.175$ and $\beta = 80$.

been the focus of the present study, is the fact that, a priori, for most situations it is impossible to determine whether the solution of the closed set of equations satisfies symmetry relation between the retarded, advanced, lesser and greater Green functions imposed by definition. For example, we have shown that for the Anderson model the relation $G_{\alpha\beta}^{<, >}(\omega) = -\left(G_{\beta\alpha}^{<, >}(\omega)\right)^*$ breaks down for a closure that is often used to describe the dynamics near the Kondo regime. We have also demonstrated that for the double Anderson model all 3 symmetry relations given by equation (15) break down for a lower level of closure. This faulty of the EOM approach leads to unphysical behavior such as complex level occupations and finite current at zero source drain bias (depending on how the current is evaluated).

We have also proposed a procedure to circumvent this deficiency by imposing symmetrization to the Green functions in such a way that all 3 symmetry relations are restored. The strength of the proposed approach is that it does not alter the GFs if symmetry is not broken. While this procedure eliminates some problems of physical importance and leads to real level occupations and vanishing current at zero source drain bias (irrespective of how the current is evaluated), certain sum rules are still violated, indicating other problems with the EOM approach. Nonetheless, the symmetrized version of the EOM technique still describes the appearance of the Kondo peak and, as will be shown in future publication provides a quantitative description of the resonant transport for the double Anderson model even in the strong inter-dot coupling limit.

VI. ACKNOWLEDGMENTS

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Supporting Information

VII. FULL DERIVATION OF THE BROKEN SYMMETRY IN THE ANDERSON MODEL

Here we present in greater detail the breakage of the relation $G_{\sigma\sigma}^<(\omega) = -(G_{\sigma\sigma}^<(\omega))^*$ described in subsection **The Anderson model** in the manuscript. We demonstrate that $G_{\sigma\sigma}^<(\omega)$ is not an imaginary function. We start by defining the following contour ordered GF:

$$G_{\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C d_\sigma(t) d_\sigma^\dagger(t') \rangle, \quad (44)$$

$$G_2(t, t') = -\frac{i}{\hbar} \langle T_C n_{\bar{\sigma}}(t) d_\sigma(t) d_\sigma^\dagger(t') \rangle, \quad (45)$$

where $\bar{\sigma}$ is the opposite spin of σ . The resulting EOMs (in Fourier space) under the approximation scheme discuss in the manuscript are:

$$(\hbar\omega - \varepsilon_\sigma - \Sigma_0(\omega)) G_{\sigma\sigma}(\omega) = 1 + U G_2(\omega), \quad (46)$$

$$G_2(\omega) = (\hbar\omega - \varepsilon_\sigma - U - \Sigma_0(\omega) - \Sigma_3(\omega))^{-1} (\langle n_{\bar{\sigma}} \rangle - \Sigma_1(\omega) G_{\sigma\sigma}(\omega)), \quad (47)$$

We define the following GFs and self-energies:

$$g(\omega) = \frac{1}{\hbar\omega - \varepsilon_\sigma - \Sigma_0(\omega)}, \quad (48)$$

$$g_2(\omega) = \frac{1}{\hbar\omega - \varepsilon_\sigma - U - \Sigma_4(\omega)}, \quad (49)$$

$$\Sigma_0(\omega) = \sum_{i,k \in \{L,R\}} \frac{|t_{k\sigma}|^2}{\hbar\omega - \varepsilon_{k,i,\sigma}}, \quad (50)$$

$$\Sigma_j(\omega) = \sum_{i,k \in \{L,R\}} A_{i,k}^{(j)} |t_{k\sigma}|^2 \left(\frac{1}{\hbar\omega + \varepsilon_{k,i,\bar{\sigma}} - \varepsilon_\sigma - \varepsilon_{\bar{\sigma}} - U} + \frac{1}{\hbar\omega - \varepsilon_{k,i,\bar{\sigma}} - \varepsilon_\sigma + \varepsilon_{\bar{\sigma}}} \right), \quad j = 1, 3 \quad (51)$$

$$\Sigma_4(\omega) = \Sigma_0(\omega) + \Sigma_3(\omega). \quad (52)$$

with $A_k^{(1)} = f_k(\varepsilon_{i,k,\sigma} - \mu_k)$, $A_k^{(3)} = 1$, and $f_k(\varepsilon_{i,k,\sigma} - \mu_k)$ is the Fermi Dirac distribution.

Rewriting the equations of the GFs in terms of the above definitions gives:

$$G_2(\omega) = g_2(\omega) \langle n_{\bar{\sigma}} \rangle - g_2(\omega) \Sigma_1(\omega) G_{\sigma\sigma}(\omega), \quad (53)$$

$$G_{\sigma\sigma}(\omega) = g(\omega) + g(\omega) U G_2(\omega), \quad (54)$$

We then merge equations (54) and (53) to get:

$$G_2(\omega) = g_2(\omega) \langle n_{\bar{\sigma}} \rangle - g_2(\omega) \Sigma_1(\omega) g(\omega) - g_2(\omega) \Sigma_1(\omega) g(\omega) U G_2(\omega). \quad (55)$$

The advanced GF can be extracted from the contour ordered one (equation (55)) by setting²⁸ $\omega \rightarrow \omega - i0^+$

$$G_2^a(\omega) = g_2^a(\omega) \langle n_{\bar{\sigma}} \rangle - g_2^a(\omega) \Sigma_1^a(\omega) g^a(\omega) - g_2^a(\omega) \Sigma_1^a(\omega) g^a(\omega) U G_2^a(\omega), \quad (56)$$

For brevity, we omit (ω) and rewrite equation (56) as:

$$G_2^a = (1 + g_2^a \Sigma_1^a g^a U)^{-1} g_2^a \langle n_{\bar{\sigma}} \rangle - (1 + g_2^a \Sigma_1^a g^a U)^{-1} g_2^a \Sigma_1^a g^a. \quad (57)$$

Define:

$$P^{r,a} = (1 + g_2^{r,a} \Sigma_1^{r,a} g^{r,a} U)^{-1}, \quad (58)$$

$$G_2^a = P^a g_2^a \langle n_{\bar{\sigma}} \rangle - P^a g_2^a \Sigma_1^a g^a, \quad (59)$$

Using Langreth theorem, the lesser projection of G_2 can be evaluated:

$$G_2^< = g_2^< \langle n_{\bar{\sigma}} \rangle - (g_2 \Sigma_1 g)^< - (g_2 \Sigma_1 g)^r U G_2^< - (g_2 \Sigma_1 g)^< U G_2^a, \quad (60)$$

with

$$g^< = g^r \Sigma_0^< g^a, \quad (61)$$

$$g_2^< = g_2^r \Sigma_4^< g_2^a, \quad (62)$$

and the lesser self energies are defined as in Ref. 34:

$$\Sigma_x^< = \Sigma_{xL}^< + \Sigma_{xR}^< = i(f_L \Gamma_{xL} + f_R \Gamma_{xR}), \quad (63)$$

where

$$\Gamma_{xk} = -2Im(\Sigma_{xk}^r), \quad (64)$$

and $\Sigma_{xk}^{r,a}$ stands for the retarded (“r”) or advanced (“a”) self-energies. Substituting equations (61) and (62) into equation (60), the lesser projection of equation (55) is given by:

$$\begin{aligned} G_2^< &= P^r g_2^< \langle n_{\bar{\sigma}} \rangle - P^r g_2^r \Sigma_1^r g^< - P^r g_2^r \Sigma_1^< g^a - P^r g_2^< \Sigma_1^a g^a \\ &\quad - P^r g_2^r \Sigma_1^r g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle - P^r g_2^r \Sigma_1^< g^a U P^a g_2^a \langle n_{\bar{\sigma}} \rangle - P^r g_2^< \Sigma_1^a g^a U P^a g_2^a \langle n_{\bar{\sigma}} \rangle \\ &\quad + P^r g_2^r \Sigma_1^r g^< U P^a g_2^a \Sigma_1^a g^a + P^r g_2^r \Sigma_1^< g^a U P^a g_2^a \Sigma_1^a g^a + P^r g_2^< \Sigma_1^a g^a U P^a g_2^a \Sigma_1^a g^a, \end{aligned} \quad (65)$$

The lesser projection of equation (54) can now be written as

$$G_{\sigma\sigma}^< = g^< + g^r U G_2^< + g^< U G_2^a. \quad (66)$$

Using our results for G_2^a and $G_2^<$ we find

$$\begin{aligned} G_{\sigma\sigma}^< &= g^< + g^r U P^r g_2^< \langle n_{\bar{\sigma}} \rangle + g^< U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle - \Sigma_1^a g^a) - g^r U P^r g_2^< \Sigma_1^a g^a \\ &\quad - g^r U P^r g_2^r (\Sigma_1^r g^< + \Sigma_1^< g^a) - g^r U P^r g_2^r \Sigma_1^r g^< U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle + \Sigma_1^a g^a) \\ &\quad - g^r U P^r g_2^r \Sigma_1^< g^a U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle + \Sigma_1^a g^a) - g^r U P^r g_2^< \Sigma_1^a g^a U P^a g_2^a (\langle n_{\bar{\sigma}} \rangle + \Sigma_1^a g^a) \end{aligned} \quad (67)$$

Applying the principle of reductio ad absurdum, we assume $G_{\sigma\sigma}^<$ is imaginary. Since it must hold for any real value of $\langle n_{\bar{\sigma}} \rangle$ between 0 and 1, we argue that the term

$$\begin{aligned} A_1 &= g^r U P^r g_2^< \langle n_{\bar{\sigma}} \rangle + g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle - g^r U P^r g_2^r \Sigma_1^r g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle \\ &\quad - g^r U P^r g_2^r \Sigma_1^< g^a U P^a g_2^a \langle n_{\bar{\sigma}} \rangle - g^r U P^r g_2^< \Sigma_1^a g^a U P^a g_2^a \langle n_{\bar{\sigma}} \rangle, \end{aligned} \quad (68)$$

is imaginary by itself. Moreover, Since A_1 must be imaginary for any value of U , the term

$$A_2 = g^r U P^r g_2^< \langle n_{\bar{\sigma}} \rangle + g^< U P^a g_2^a \langle n_{\bar{\sigma}} \rangle, \quad (69)$$

should be imaginary as well. Using the fact that U and $\langle n_{\bar{\sigma}} \rangle$ are real quantities and by definition $g_2^<$ and $g^<$ are imaginary, for A_2 to be imaginary, one requires that its real part vanishes, i.e.,:

$$Im(g^r P^r) g_2^< + Im(P^a g_2^a) g^< = 0. \quad (70)$$

In other words the equality

$$\text{Im}(g^r P^r) g_2^r \Sigma_4^< g_2^a = -\text{Im}(P^a g_2^a) g^r \Sigma_0^< g^a, \quad (71)$$

must hold for the assumption that $G_{\sigma\sigma}^<$ is imaginary to be satisfied. Using the definitions for g and g_2 the last equality can be rewritten as:

$$\text{Im}(g^r P^r) \frac{-if(\omega) \text{Im}(\Sigma_4^r)}{(\hbar\omega - \varepsilon_4 - U)^2 + (\text{Im}(\Sigma_4^r))^2} = \text{Im}(P^a g_2^a) \frac{if(\omega) \text{Im}(\Sigma_0^r)}{(\hbar\omega - \varepsilon_0)^2 + (\text{Im}(\Sigma_0^r))^2}, \quad (72)$$

where $\varepsilon_0 = \varepsilon_\sigma + \text{Re}(\Sigma_0^r)$ and $\varepsilon_4 = \varepsilon_\sigma + \text{Re}(\Sigma_4^r)$. Starting with the L.H.S. of equation (72), we look at $g^r P^r$

$$\begin{aligned} g^r P^r &= \frac{g^r}{1 + g_2^r \Sigma_1^r g^r U} = \frac{1}{\hbar\omega - \varepsilon_\sigma - \Sigma_0^r + \frac{\Sigma_1^r U}{\hbar\omega - \varepsilon_\sigma - U - \Sigma_4^r}} \\ &= \frac{\hbar\omega - \varepsilon_\sigma - U - \Sigma_4^r}{(\hbar\omega - \varepsilon_\sigma - \Sigma_0^r)(\hbar\omega - \varepsilon_\sigma - U - \Sigma_4^r) + \Sigma_1^r U} \\ &= \frac{\hbar\omega - \varepsilon_4 - U - i(\text{Im}\Sigma_4^r)}{(\hbar\omega - \varepsilon_0 - i(\text{Im}\Sigma_0^r))(\hbar\omega - \varepsilon_4 - U - i(\text{Im}\Sigma_4^r)) + U \cdot \text{Re}(\Sigma_1^r) + U \cdot i(\text{Im}\Sigma_1^r)}. \end{aligned} \quad (73)$$

Denote $a_0 = \hbar\omega - \varepsilon_0$, $a_1 = \text{Re}(\Sigma_1^r)$, $a_4 = \hbar\omega - \varepsilon_4 - U$ and $b_x = \text{Im}(\Sigma_x^r)$ with $x = 0, 1, 4$

$$\begin{aligned} g^r P^r &= \frac{a_4 - ib_4}{(a_0 - ib_0)(a_4 - ib_4) + Ua_1 + iUb_1} \\ &= \frac{a_4 - ib_4}{a_0a_4 - b_0b_4 + Ua_1 - i(a_0b_4 + a_4b_0 - Ub_1)}. \end{aligned} \quad (74)$$

Denote $D = a_0a_4 - b_0b_4 + Ua_1$ and $E = a_0b_4 + a_4b_0 - Ub_1$, so we can rewrite equation (74) as

$$g^r P^r = \frac{a_4 - ib_4}{D - iE} = \frac{(a_4 - ib_4)(D + iE)}{D^2 + E^2} = \frac{a_4D + b_4E - i(b_4D - a_4E)}{D^2 + E^2}. \quad (75)$$

Finally

$$\text{Im}(g^r P^r) = -\frac{b_4D - a_4E}{D^2 + E^2} \quad (76)$$

The L.H.S. of equation (72) is thus

$$\text{Im}(g^r P^r) \frac{-if(\omega) \text{Im}(\Sigma_4^r)}{(\hbar\omega - \varepsilon_4 - U)^2 + (\text{Im}(\Sigma_4^r))^2} = \frac{if(\omega) b_4}{(a_4)^2 + (b_4)^2} \frac{b_4D - a_4E}{D^2 + E^2}. \quad (77)$$

Now we turn to analyze the R.H.S. of equation (72). We start with evaluating $P^a g_2^a$

$$\begin{aligned} P^a g_2^a &= \frac{g_2^a}{1 + g_2^a \Sigma_1^a g^a U} = \frac{1}{\hbar\omega - \varepsilon_\sigma - U - \Sigma_4^a + \frac{\Sigma_1^a U}{\hbar\omega - \varepsilon_\sigma - \Sigma_0^a}} \\ &= \frac{\hbar\omega - \varepsilon_\sigma - \Sigma_0^a}{(\hbar\omega - \varepsilon_\sigma - U - \Sigma_4^a)(\hbar\omega - \varepsilon_\sigma - \Sigma_0^a) + \Sigma_1^a U} \\ &= \frac{a_0 + ib_0}{(a_0 + ib_0)(a_4 + ib_4) + Ua_1 - iUb_1} \\ &= \frac{a_0 + ib_0}{a_0a_4 - b_0b_4 + Ua_1 + i(a_0b_4 + a_4b_0 - Ub_1)} \\ &= \frac{a_0 + ib_0}{D + iE} = \frac{(a_0 + ib_0)(D - iE)}{D^2 + E^2} = \frac{a_0D + b_0E + i(b_0D - a_0E)}{D^2 + E^2}. \end{aligned} \quad (78)$$

To go from the second line to the third line in equation (78) we used $\text{Im}(\Sigma_x^r) = -\text{Im}(\Sigma_x^a)$. Finally:

$$\text{Im}(P^a g_2^a) = \frac{b_0D - a_0E}{D^2 + E^2}. \quad (79)$$

The R.H.S. of equation (72) is thus,

$$\text{Im}(P^a g_2^a) \frac{if(\omega) \text{Im}(\Sigma_0^r)}{(\hbar\omega - \varepsilon_0)^2 + (\text{Im}(\Sigma_0^r))^2} = \frac{b_0 D - a_0 E}{D^2 + E^2} \frac{if(\omega) b_0}{(a_0)^2 + (b_0)^2}. \quad (80)$$

The equality (equation(72)) now reads:

$$\frac{b_4}{(a_4)^2 + (b_4)^2} \frac{b_4 D - a_4 E}{D^2 + E^2} = \frac{b_0 D - a_0 E}{D^2 + E^2} \frac{b_0}{(a_0)^2 + (b_0)^2}, \quad (81)$$

or

$$\frac{b_4^2 D - a_4 b_4 E}{(a_4)^2 + (b_4)^2} = \frac{b_0^2 D - a_0 b_0 E}{(a_0)^2 + (b_0)^2}. \quad (82)$$

Substituting $D = a_0 a_4 - b_0 b_4 + U a_1$ and $E = a_0 b_4 + a_4 b_0 - U b_1$ one can easily show that the equality **does not hold**. Thus, $G_{\sigma\sigma}^<(\omega)$ is not an imaginary function as it should be by definition.

In the paper we argued that a simpler closure (as used for example, in Ref. 32) will not violate the symmetries of the GFs. In what follows we show that under the simpler closure, indeed, $G_{\sigma\sigma}^<(\omega) = -(G_{\sigma\sigma}^<(\omega))^*$. Our starting point is the same. Define the contour ordered GFs:

$$G_{\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C d_\sigma(t) d_\sigma^\dagger(t') \rangle, \quad (83)$$

$$G_2(t, t') = -\frac{i}{\hbar} \langle T_C n_{\bar{\sigma}}(t) d_\sigma(t) d_\sigma^\dagger(t') \rangle, \quad (84)$$

Following the approximations of Ref. 32, the resulting EOMs (in Fourier space) are:

$$(\hbar\omega - \varepsilon_\sigma - \Sigma_0(\omega)) G_{\sigma\sigma}(\omega) = 1 + U G_2(\omega), \quad (85)$$

$$G_2(\omega) = (\hbar\omega - \varepsilon_\sigma - U - \Sigma_0(\omega))^{-1} \langle n_{\bar{\sigma}} \rangle. \quad (86)$$

We define

$$g(\omega) = \frac{1}{\hbar\omega - \varepsilon_\sigma - \Sigma_0(\omega)}, \quad (87)$$

$$g_2(\omega) = \frac{1}{\hbar\omega - \varepsilon_\sigma - U - \Sigma_0(\omega)}, \quad (88)$$

$$\Sigma_0(\omega) = \sum_{i,k \in \{L,R\}} \frac{|t_{k\sigma}|^2}{\hbar\omega - \varepsilon_{k,i,\sigma}}. \quad (89)$$

Rewriting equations (85) and (86) in terms of the given definitions we get:

$$G_2(\omega) = g_2(\omega) \langle n_{\bar{\sigma}} \rangle, \quad (90)$$

$$G_{\sigma\sigma}(\omega) = g(\omega) + g(\omega) U G_2(\omega), \quad (91)$$

Substitute equation (90) into equation (91)

$$G_{\sigma\sigma}(\omega) = g(\omega) + g(\omega) U \langle n_{\bar{\sigma}} \rangle g_2(\omega). \quad (92)$$

Applying the Langreth rules we find the lesser GF (omitting (ω) for brevity):

$$G_{\sigma\sigma}^< = g^< + g^r U \langle n_{\bar{\sigma}} \rangle g_2^< + g^< U \langle n_{\bar{\sigma}} \rangle g_2^a \quad (93)$$

where $g^< = g^r \Sigma_0^< g^a$, $g_2^< = g_2^r \Sigma_0^< g_2^a$, and $\Sigma_0^<$ is defined in equations (63) and (64). By definition $g^<$ is imaginary, hence, for $G_{\sigma\sigma}^<$ to be imaginary one requires that

$$A_1 = g^r U \langle n_{\bar{\sigma}} \rangle g_2^r \Sigma_0^< g_2^a + g^r \Sigma_0^< g^a U \langle n_{\bar{\sigma}} \rangle g_2^a, \quad (94)$$

be imaginary. Since $g_2^r \Sigma_0^< g_2^a$ and $g^r \Sigma_0^< g^a$ are pure imaginary quantities, for $G_{\sigma\sigma}^<$ to be pure imaginary, the real part of A_1 needs to cancel, i.e.,:

$$\text{Im}(g^r) g_2^r \Sigma_0^< g_2^a = -\text{Im}(g_2^a) g^r \Sigma_0^< g^a. \quad (95)$$

Define

$$\varepsilon_0 = \varepsilon_{\sigma} + \text{Re}(\Sigma_0^r), \quad (96)$$

$$\Gamma = -\text{Im}(\Sigma_0^r), \quad (97)$$

and use it to rewrite the equation (95) as:

$$\frac{\Gamma}{(\hbar\omega - \varepsilon_0)^2 + (\Gamma)^2} \Sigma_0^< \frac{1}{(\hbar\omega - \varepsilon_0 - U)^2 + (\Gamma)^2} = -\frac{-\Gamma}{(\hbar\omega - \varepsilon_0 - U)^2 + (\Gamma)^2} \Sigma_0^< \frac{1}{(\hbar\omega - \varepsilon_0)^2 + (\Gamma)^2}. \quad (98)$$

Obviously the real part of A_1 cancels, hence $G_{\sigma\sigma}^<$ is imaginary and fulfills the symmetry $G_{\sigma\sigma}^<(\omega) = -(G_{\sigma\sigma}^<(\omega))^*$.

VIII. FULL DERIVATION OF THE BROKEN SYMMETRY IN THE DOUBLE ANDERSON MODEL

Now we refer to subsection **The double Anderson model** in the manuscript. In what follows we show in greater detail that $(G_{\alpha\beta}^{\sigma\sigma}(\omega))^r \neq ((G_{\beta\alpha}^{\sigma\sigma}(\omega))^a)^*$. Again, following the derivation in Ref. 50 we define the following contour ordered GFs:

$$G_{\alpha\beta}^{\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C d_{\alpha\sigma}(t) d_{\beta\sigma}^\dagger(t') \rangle, \quad (99)$$

$$\mathbb{G}_{\alpha\beta\gamma}^{\tau\sigma\sigma}(t, t') = -\frac{i}{\hbar} \langle T_C n_{\alpha\tau}(t) d_{\beta\sigma}(t) d_{\gamma\sigma}^\dagger(t') \rangle. \quad (100)$$

where $\tau = \sigma/\bar{\sigma}$. The resulting EOM are:

$$\begin{aligned} G_{\alpha\beta}^{\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha,\sigma} - \Sigma_0(\omega))^{-1} \times (\delta_{\alpha\beta}^{\sigma\sigma} + h_{\alpha\beta}^{\sigma} G_{\beta\beta}^{\sigma\sigma}(\omega) + U_{\alpha} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) \\ &\quad + V_{\alpha\beta}^{\sigma\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\alpha\beta}^{\sigma\sigma} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega)), \end{aligned} \quad (101)$$

$$\begin{aligned} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha\sigma} - U_{\alpha} - V_{\alpha\beta}^{\sigma\sigma} \langle n_{\beta\sigma} \rangle - V_{\alpha\beta}^{\sigma\bar{\sigma}} \langle n_{\beta\bar{\sigma}} \rangle - \Sigma_0(\omega))^{-1} \\ &\quad \times [h_{\alpha\beta}^{\sigma} \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\alpha\bar{\sigma}} \rangle (V_{\alpha\beta}^{\sigma\sigma} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega) + V_{\alpha\beta}^{\sigma\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \\ \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\beta\sigma} - U_{\beta} \langle n_{\beta\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\sigma} \langle n_{\alpha\sigma} \rangle - V_{\beta\alpha}^{\sigma\bar{\sigma}} - \Sigma_0(\omega))^{-1} \\ &\quad \times [\langle n_{\alpha\bar{\sigma}} \rangle + h_{\beta\alpha}^{\sigma} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\alpha\bar{\sigma}} \rangle (U_{\beta} \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\beta\alpha}^{\sigma\sigma} \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega))], \\ \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\beta\sigma} - U_{\beta} \langle n_{\beta\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\bar{\sigma}} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\sigma} - \Sigma_0(\omega))^{-1} \\ &\quad \times [\langle n_{\alpha\sigma} \rangle + h_{\beta\alpha}^{\sigma} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\alpha\sigma} \rangle (U_{\beta} \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\beta\alpha}^{\sigma\bar{\sigma}} \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \\ \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha\sigma} - U_{\alpha} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\alpha\beta}^{\sigma\sigma} \langle n_{\beta\sigma} \rangle - V_{\alpha\beta}^{\sigma\bar{\sigma}} - \Sigma_0(\omega))^{-1} \\ &\quad \times [h_{\alpha\beta}^{\sigma} \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\beta\bar{\sigma}} \rangle (U_{\alpha} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\alpha\beta}^{\sigma,\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega))], \\ \mathbb{G}_{\beta\alpha\beta}^{\sigma\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\alpha\sigma} - U_{\alpha} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\alpha\beta}^{\sigma\bar{\sigma}} \langle n_{\beta\bar{\sigma}} \rangle - V_{\alpha\beta}^{\sigma\sigma} - \Sigma_0(\omega))^{-1} \\ &\quad \times [-\langle d_{\beta\sigma}^\dagger d_{\alpha,\sigma} \rangle + h_{\alpha\beta}^{\sigma} \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega) + \langle n_{\beta,\sigma} \rangle (U_{\alpha} \mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + V_{\alpha,\beta}^{\sigma,\bar{\sigma}} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \\ \mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega) &= (\hbar\omega - \varepsilon_{\beta\sigma} - U_{\beta} - V_{\beta\alpha}^{\sigma\bar{\sigma}} \langle n_{\alpha\bar{\sigma}} \rangle - V_{\beta\alpha}^{\sigma\sigma} \langle n_{\alpha\sigma} \rangle - \Sigma_0(\omega))^{-1} \\ &\quad \times [\langle n_{\beta\bar{\sigma}} \rangle + h_{\beta\alpha}^{\sigma} \mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma}(\omega) + \langle n_{\beta\bar{\sigma}} \rangle (V_{\beta\alpha}^{\sigma,\bar{\sigma}} \mathbb{G}_{\alpha\beta\beta}^{\sigma\sigma\sigma}(\omega) + V_{\beta\alpha}^{\sigma\bar{\sigma}} \mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma}(\omega))], \end{aligned} \quad (102)$$

By applying the Langreth rules one can find the retarded and advanced projections of the single particle GF (equation (101)). For simplicity we derive them for the case where $V_{ij}^{\sigma\tau} = 0$. Define (as usual omitting (ω) for brevity)

$$(g_i)^{r,a} = \frac{1}{\hbar\omega - \varepsilon_{i,\sigma} - \Sigma_0^{r,a}}, \quad (103)$$

$$(g_{ii}^{\bar{\sigma}\sigma})^{r,a} = \frac{1}{\hbar\omega - \varepsilon_{i,\sigma} - U_i - \Sigma_0^{r,a}}, \quad (104)$$

$$(g_{ij}^{\bar{\sigma}\sigma})^{r,a} = \frac{1}{\hbar\omega - \varepsilon_{j,\sigma} - U_j \langle n_{j,\bar{\sigma}} \rangle - \Sigma_0^{r,a}}, \quad (105)$$

where Σ_0 is defined in equation (50). Now we are ready to look at the equation we get for $\left(G_{\alpha\beta}^{\sigma\sigma}(\omega)\right)^r$.

$$(G_{\alpha\beta}^{\sigma\sigma})^r = (g_\alpha)^r h_{\alpha,\beta}^\sigma (G_{\beta\beta}^{\sigma\sigma})^r + (g_\alpha)^r U_\alpha (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r, \quad (106)$$

$$(G_{\beta\beta}^{\sigma\sigma})^r = (g_\beta)^r + (g_\beta)^r h_{\beta,\alpha}^\sigma (G_{\alpha\beta}^{\sigma\sigma})^r + (g_\beta)^r U_\beta (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r, \quad (107)$$

$$(\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r = (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (\mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma})^r, \quad (108)$$

$$(\mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r = (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^\sigma (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r + (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_\alpha (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r, \quad (109)$$

$$(\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r = (g_{\beta\beta}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle + (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (\mathbb{G}_{\beta\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r, \quad (110)$$

$$(\mathbb{G}_{\alpha\beta\beta}^{\bar{\sigma}\sigma\sigma})^r = (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle + (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r + (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle U_\beta (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r. \quad (111)$$

Substituting $\left(G_{\beta\beta}^{\sigma\sigma}\right)^r$ into the equation of $\left(G_{\alpha\beta}^{\sigma\sigma}\right)^r$:

$$(G_{\alpha\beta}^{\sigma\sigma})^r = (g_\alpha)^r h_{\alpha,\beta}^\sigma \left((g_\beta)^r + (g_\beta)^r h_{\beta,\alpha}^\sigma (G_{\alpha\beta}^{\sigma\sigma})^r + (g_\beta)^r U_\beta (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r \right) + (g_\alpha)^r U_\alpha (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r, \quad (112)$$

$$\begin{aligned} (G_{\alpha\beta}^{\sigma\sigma})^r &= (I - (g_\alpha)^r h_{\alpha,\beta}^\sigma (g_\beta)^r h_{\beta,\alpha}^\sigma)^{-1} \\ &\times \left((g_\alpha)^r h_{\alpha,\beta}^\sigma (g_\beta)^r + (g_\alpha)^r h_{\alpha,\beta}^\sigma (g_\beta)^r U_\beta (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r + (g_\alpha)^r U_\alpha (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r \right). \end{aligned} \quad (113)$$

Now we need the equations for $\left(\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma}\right)^r$ and $\left(\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma}\right)^r$. Using equations (108) to (111) we get:

$$\begin{aligned} (\mathbb{G}_{\alpha\alpha\beta}^{\bar{\sigma}\sigma\sigma})^r &= (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle U_\beta \\ &\times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^\sigma)^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_\alpha)^{-1} \\ &\times ((g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle + (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle U_\beta \\ &\times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^\sigma)^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle), \end{aligned} \quad (114)$$

and

$$\begin{aligned} (\mathbb{G}_{\beta\beta\beta}^{\bar{\sigma}\sigma\sigma})^r &= (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha\beta}^\sigma - (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_\alpha \\ &\times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma)^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle U_\beta)^{-1} \\ &\times ((g_{\beta\beta}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle + (g_{\beta\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^r \langle n_{\beta\bar{\sigma}} \rangle U_\alpha \\ &\times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r h_{\beta\alpha}^\sigma)^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^r h_{\alpha,\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \langle n_{\alpha,\bar{\sigma}} \rangle). \end{aligned} \quad (115)$$

The same way one can derive an expression for $(G_{\beta\alpha}^{\sigma\sigma})^a$

$$(G_{\beta\alpha}^{\sigma\sigma})^a = (I - (g_\beta)^a h_{\beta,\alpha}^\sigma (g_\alpha)^a h_{\alpha,\beta}^\sigma)^{-1} \times ((g_\beta)^a h_{\beta,\alpha}^\sigma (g_\alpha)^a + (g_\beta)^a h_{\beta,\alpha}^\sigma (g_\alpha)^a U_\alpha (\mathbb{G}_{\alpha\alpha}^{\bar{\sigma}\sigma})^a + (g_\beta)^a U_\beta (\mathbb{G}_{\beta\beta}^{\bar{\sigma}\sigma})^a), \quad (116)$$

with

$$\begin{aligned} (\mathbb{G}_{\beta\beta}^{\bar{\sigma}\sigma})^a &= (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta,\bar{\sigma}} \rangle U_\alpha \\ &\quad \times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^\sigma)^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle U_\beta)^{-1} \\ &\quad \times ((g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta,\bar{\sigma}} \rangle + (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta,\bar{\sigma}} \rangle U_\alpha \\ &\quad \times (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^\sigma)^{-1} (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle), \end{aligned} \quad (117)$$

and

$$\begin{aligned} (\mathbb{G}_{\alpha\alpha}^{\bar{\sigma}\sigma})^a &= (1 - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a h_{\beta\alpha}^\sigma - (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle U_\beta \\ &\quad \times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma)^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta,\bar{\sigma}} \rangle U_\alpha)^{-1} \\ &\quad \times ((g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle + (g_{\alpha\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma (g_{\alpha\beta}^{\bar{\sigma}\sigma})^a \langle n_{\alpha\bar{\sigma}} \rangle U_\beta \\ &\quad \times (1 - (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a h_{\alpha\beta}^\sigma)^{-1} (g_{\beta\beta}^{\bar{\sigma}\sigma})^a h_{\beta,\alpha}^\sigma (g_{\beta\alpha}^{\bar{\sigma}\sigma})^a \langle n_{\beta,\bar{\sigma}} \rangle). \end{aligned} \quad (118)$$

The question we now ask is whether

$$(G_{\alpha\beta}^{\sigma\sigma})^r = ((G_{\beta\alpha}^{\sigma\sigma})^a)^*. \quad (119)$$

Using

$$(g_i)^r = ((g_i)^a)^*, \quad (g_{ii}^2)^r = ((g_{ii}^2)^a)^*, \quad (g_{ij}^2)^r = ((g_{ij}^2)^a)^*, \quad (120)$$

and looking back at equations (113) and (116) we find that

$$(I - (g_\alpha)^r h_{\alpha,\beta}^\sigma (g_\beta)^r h_{\beta,\alpha}^\sigma)^{-1} = \left((I - (g_\beta)^a h_{\beta,\alpha}^\sigma (g_\alpha)^a h_{\alpha,\beta}^\sigma)^{-1} \right)^*, \quad (121)$$

and that

$$(g_\alpha)^r h_{\alpha,\beta}^\sigma (g_\beta)^r = ((g_\beta)^a h_{\beta,\alpha}^\sigma (g_\alpha)^a)^*. \quad (122)$$

Therefore, it is sufficient check whether the next equality

$$(g_\alpha)^r U_\alpha (\mathbb{G}_{\alpha\alpha}^{\bar{\sigma}\sigma})^r + (g_\alpha)^r h_{\alpha,\beta}^\sigma (g_\beta)^r U_\beta (\mathbb{G}_{\beta\beta}^{\bar{\sigma}\sigma})^r = ((g_\beta)^a h_{\beta,\alpha}^\sigma (g_\alpha)^a U_\alpha (\mathbb{G}_{\alpha\alpha}^{\bar{\sigma}\sigma})^a + (g_\beta)^a U_\beta (\mathbb{G}_{\beta\beta}^{\bar{\sigma}\sigma})^a)^*, \quad (123)$$

holds. Substitute the equations for $(\mathbb{G}_{\alpha\alpha}^{\bar{\sigma}\sigma})^r$, $(\mathbb{G}_{\beta\beta}^{\bar{\sigma}\sigma})^r$, $(\mathbb{G}_{\alpha\alpha}^{\bar{\sigma}\sigma})^a$ and $(\mathbb{G}_{\beta\beta}^{\bar{\sigma}\sigma})^a$ into equation (123) and after some tedious algebra we find that unless

$$(g_{\alpha\beta}^{\bar{\sigma}\sigma})^r = ((g_\beta)^a)^* = (g_\beta)^r, \quad (124)$$

the identity $(G_{\alpha\beta}^{\sigma\sigma})^r = ((G_{\beta\alpha}^{\sigma\sigma})^a)^*$ does not hold. But as

$$(g_{\alpha\beta}^{\bar{\sigma}\sigma})^r = \frac{1}{\hbar\omega - \varepsilon_{\beta,\sigma} - U_\beta \langle n_{\beta,\bar{\sigma}} \rangle - \Sigma_0^r}, \quad (125)$$

and

$$(g_\beta)^r = \frac{1}{\hbar\omega - \varepsilon_{\beta,\sigma} - \Sigma_0^r}, \quad (126)$$

it is obvious that $(g_{\alpha\beta}^{\bar{\sigma}\sigma})^r \neq ((g_\beta)^a)^*$, hence finally $(G_{\alpha\beta}^{\sigma\sigma})^r \neq ((G_{\beta\alpha}^{\sigma\sigma})^a)^*$. The same can be done to show that $(G_{\alpha\beta}^{\sigma\sigma})^{<, >} \neq - \left((G_{\beta\alpha}^{\sigma\sigma})^{<, >} \right)^*$ and $(G_{\alpha\beta}^{\sigma\sigma})^r - (G_{\alpha\beta}^{\sigma\sigma})^a \neq (G_{\alpha\beta}^{\sigma\sigma})^{>} - (G_{\alpha\beta}^{\sigma\sigma})^{<}$.
